

On the notion of quantum Lyapunov exponent.

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Abstract. Classical chaos refers to the property of trajectories to diverge exponentially as time $t \rightarrow \infty$. It is characterized by a positive Lyapunov exponent.

There are many different descriptions of quantum chaos. The one related to the notion of generalized (quantum) Lyapunov exponent is based either on qualitative physical considerations or on the so-called symplectic tomography map [1, 2].

The purpose of this note is to show how the definition of quantum Lyapunov exponent naturally arises in the framework of the Moyal phase space formulation of quantum mechanics [3], and is based on the notions of quantum trajectories and the family of quantizers [4]. The role of the Heisenberg uncertainty principle in the statement of the criteria for quantum chaos is made explicit.

1. Introduction.

Irregular behaviour of classical dynamical systems arising from deterministic time evolution without any external randomness and stochasticity – the so called deterministic chaos – manifests itself as an extremely sensitive dependence on the initial conditions, which makes unstable the long-time prediction of the dynamics.

In such a system, a positive Lyapunov exponent is a quantitative measure of the infinite time exponential separation of neighbouring orbits.

In detail, let the system have a form $\dot{x} = F(x)$, where $x = (q, p)$ is d -dimensional vector from the system's phase space. Denote by $x(t, x_0)$ its solution with initial point at x_0 and $t \in (0, \infty)$. Then the Lyapunov exponent is given by

$$\lambda = \lim_{t \rightarrow \infty} \frac{1}{t} \ln \frac{\|\delta x(t)\|}{\|\delta x(0)\|}.$$

Here $\|\cdot\|$ represents the d -dimensional Euclidian norm, and $\|\delta x(0)\|$ is initial infinitesimal deviation from x_0 , $\|\delta x(t)\| = \|x(t, x_0 + \delta x(0)) - x(t, x_0)\|$ is

deviation from $x(t, x_0)$ at time t . In the limit $\|\delta x(0)\| \rightarrow 0$ one obtains

$$\lambda_v = \lim_{t \rightarrow \infty} \frac{1}{t} \ln [(v \cdot \nabla_{x_0}) x(t, x_0)], \quad (1)$$

where $v \in R^d$ is a unit vector in the direction of the initial displacement, $\delta x(0)$, and ∇_{x_0} is gradient w.r.t. the initial point x_0 .

To extend this notion to quantum mechanics it is natural to use its phase space formulation where quantum observables on the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^n, \mathbb{C})$ are represented by functions on the phase space, called symbols. Consider Weyl symbol $A(x)$, obtained from the operator \hat{A} s.t. $\hat{A}\psi(q') \equiv \int \langle q' | \hat{A} | q'' \rangle \langle q'' | \psi \rangle dq''$, $\psi \in \mathcal{H}$, by formula

$$A(x) = 2^n \int e^{2ips/\hbar} \langle q - s | \hat{A} | q + s \rangle ds \equiv [\hat{A}]_w(x). \quad (2)$$

The dimension of the phase space is even, $d = 2n$.

In this case quantum mechanical mean value

$$\langle \hat{A} \rangle_\rho = \text{Tr } \hat{A} \hat{\rho} = \int \langle q' | \hat{A} | q'' \rangle \langle q'' | \hat{\rho} | q' \rangle dq' dq'' \quad (3)$$

can be written in a form analogous to classical statistical mechanics

$$\langle \hat{A} \rangle_\rho = \int A(x) W(x) dx, \quad (4)$$

which gives mean value of A in the state $\rho(x) = [\hat{\rho}]_w(x)$. Here W is the Wigner distribution function $W(x) = h^{-n} \rho(x)$.

One drawback of this approach, relative to the classical statistical density, is that the $W(x)$ is not everywhere nonnegative so is not a conventional probability density.

To circumvent this difficulty another representation can be considered in which a new density is defined as the Radon transform [5] of the Wigner function $W(x)$. It takes only non-negative values and becomes straightforward analog of the classical statistical density. In [6] it was shown that the tomographic representation of quantum mechanics based on Radon transform is an alternative to the Weyl–Wigner formalism.

Due to their similar nature in quantum and classical cases the tomographic distributions were used in [2] to define a quantum Lyapunov exponent. In detail, let $U(t) = \exp[-it\hat{H}/\hbar]$ be the Schrödinger unitary evolution operator, and $\hat{X}(t) = U^\dagger(t) \hat{x} U(t)$ be time evolution of the quantum coordinate operators $\hat{x} = (\hat{p}, \hat{q})$. The formula for quantum Lyapunov exponent turned out to be

$$\Lambda_v = \lim_{t \rightarrow \infty} \frac{1}{t} \ln \|\langle \hat{X}(t) \rangle_{\rho_0^v}\|, \quad (5)$$

where average is taken with respect to a special initial singular density $\hat{\rho}_0^v$, the kernel of which has the form

$$\langle q' | \hat{\rho}_0^v | q'' \rangle = e^{ip_0(q' - q'')/\hbar} \left((v_1 \nabla) + \frac{iv_2(q' - q'')}{\hbar} \right) \delta \left(q_0 - \frac{q' + q''}{2} \right). \quad (6)$$

Here parameters (q_0, p_0) correspond to the initial point x_0 in the phase space, and vector $v = (v_1, v_2) \in \mathbb{R}^d$ defines the direction of the initial deviation from x_0 . The authors of [2] stress special role of the tomographic distributions for obtaining these formulas, in particular the one for the initial density (6). In [1] similar formula is obtained from qualitative considerations but the choice of the initial density appears rather *ad hoc* in the quantum mechanical setting. As it is shown in [1][2], quantum Lyapunov exponent (5,6) helps to classify different types of quantum complexity. There are examples where exponential rate of growth for the trace $\langle \hat{X}(t) \rangle_{\rho_0^v} = \text{Tr} \hat{X}(t) \hat{\rho}_0^v$ of position and momentum observables starting from the singular initial density matrix (6) was found in quantum mechanics. In many cases when quantum mechanics has damping effect on the classical chaos and the rate of growth for the trace is milder than exponential, the notion of quantum sensitive dependence was used instead.

In this paper we derive representations of the quantum Lyapunov index from the Weyl–Stratonovich quantizer [4]. Using notion of quantum trajectory [3], i.e. the symbol of operator $\hat{X}(t)$, we rewrite the formula for quantum Lyapunov exponent in the form identical to the classical definition (1) (see formula (24)), replacing classical trajectory $x(t, x_0)$ with quantum trajectory $X(x_0, t; \hbar)$. In this form it becomes transparent that the definition respects the correspondence principle: in the limit $\hbar \rightarrow 0$ definition of quantum Lyapunov exponent transforms into the classical one. In contrast to the classical trajectory, the Heisenberg uncertainty principle prevents the quantum trajectory to be interpreted as a measurable physical value despite the fact that it can be viewed as a limit of a sequence of quantum means.

2. Quantum Phase Space. Weyl–Stratonovich quantizer.

Development of phase space formulation of quantum mechanics has a long history, but it still is of interest due to extensive study of possible generalizations to the case of non-Abelian gauge theory with support on a Riemannian manifold.

In 1932 Wigner introduced his quasi-probability distribution associated with the wave function $\psi(q)$

$$W(x) = \left(\frac{2}{\hbar} \right)^n \int e^{2ips/\hbar} \psi^+(q - s) \psi(q + s) ds, \quad \hbar = 2\pi\hbar. \quad (7)$$

Further developing Groenewold's ideas published in 1946, Moyal gave in his paper of 1949 statistical interpretation of the Wigner's formula as a Fourier inverse of the expectation value of the Heisenberg translation operator

$$T(y) \equiv \exp(-2iJy \cdot \hat{x}/\hbar), \quad T(x)^+ \hat{x} T(x) = \hat{x} - 2xI. \quad (8)$$

namely

$$W(x) = \left(\frac{2}{\hbar}\right)^{2n} \int e^{2ix \cdot Jy/\hbar} \langle \psi | T(y) | \psi \rangle dy.$$

where J denotes the Poisson matrix $\begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$. He also showed that the Wigner rule (7) of getting the phase space function from the operator $|\psi\rangle\langle\psi|$ (and \hat{A}) is inverse to the Weyl quantization rule,

$$\langle q' | \hat{A} | q'' \rangle = h^{-n} \int e^{ip(q' - q'')/\hbar} A\left(\frac{q' + q''}{2}, p\right) dp. \quad (9)$$

A significant step further was the introduction [4, 7, 8] of the family of unitary operators $\Delta(x)$ labelled by points of the phase space. These operators define both quantization (9) and dequantization (2) rules, which establishes a unitary isomorphism between symbols and operators,

$$A(x) = 2^n \text{Tr} \Delta(x) \hat{A}, \quad \hat{A} = \int A(x) \Delta(x) d^*x. \quad (10)$$

For this reason the operators $\Delta(x)$ are called quantizers. Above $d^*x = (\pi\hbar)^{-n} dx$ denotes a dimensionless phase space measure.

The fundamental nature of quantizers also reveals itself in the fact that they define the noncommutative product $*$ for the phase space functions

$$(A * B)(x) = \int A(y) B(z) K(x, y, z) dy dz, \quad (11)$$

$$K(x, y, z) = \frac{2^n}{(\pi\hbar)^{2n}} \text{Tr} \Delta(x) \Delta(y) \Delta(z). \quad (12)$$

Other useful properties [9] of quantizers are:

1. $\Delta(x) = \Delta(x)^+ = \Delta(x)^{-1}$. Thus $\Delta(x)^2 = I$ and $||\Delta(x)|| = 1$;
2. $\text{Tr} \Delta(x) = 2^{-n}$;
3. $\text{Tr} [\Delta(x) \Delta(x')] = (\pi\hbar/2)^n \delta(x - x')$;
4. $\Delta(x) = \int e^{2ix \cdot Jy/\hbar} T(y) d^*y$;

5. $\rho(x) = 2^n \langle \psi | \Delta(x) | \psi \rangle$;
6. $\Delta(0) \hat{x} \Delta(0) = -\hat{x}$;
7. $\Delta(x) = T(x/2)^+ \Delta(0) T(x/2)$;
8. $\int \Delta(x) d^*x = I$.

Many authors (see e.g. [10]) use quantizers as a fundamental object defining the deformation quantization introduced in 1978 by Bayen et al [11].

There is one observation useful for the purpose of our note. In view of the 1st equation of (10) Property 3 tells us that the symbol of the quantizer is $[\Delta(x)]_w(x') = (h/2)^n \delta(x - x')$, and by (9) that its kernel is

$$\langle q' | \Delta(x) | q'' \rangle = 2^{-n} e^{ip(q' - q'')/\hbar} \delta\left(q - \frac{q' + q''}{2}\right). \quad (13)$$

An attractive feature of quantum phase space is computation of the trace of an operator and pairs of operators. For an operators \hat{A}, \hat{B} with symbols $A(x), B(x)$ one has

$$\text{Tr } \hat{A} = \frac{1}{h^n} \int A(x) dx, \quad (14)$$

$$\text{Tr } \hat{A} \hat{B} = \frac{1}{h^n} \int A * B(x) dx = \frac{1}{h^n} \int A(x) B(x) dx. \quad (15)$$

Identity (14) follows from (10) and Property 2. The removal of the $*$ operation in (15) is a consequence of Properties 3 and 8.

3. Quantum means and symbols.

Mean value of a quantum observable given by operator \hat{A} in a unit normalized quantum state $\psi(q)$ is

$$\langle \psi | \hat{A} | \psi \rangle = \text{Tr } \hat{A} \hat{\rho}, \quad \hat{\rho} = |\psi\rangle \langle \psi|. \quad (16)$$

This is an example of formula (3) for the pure state density. Its phase space form is (4) which is a special case of the trace identity (15).

Let us consider a family of Gaussian states localized near $q = q_0 \in R^n$ with width $\sqrt{\hbar}$

$$\psi_{\hbar}(q; q_0, p_0) = \frac{1}{(\pi \hbar)^{n/4}} \exp\left(-\frac{(q - q_0)^2}{2\hbar} + \frac{i}{\hbar} p_0(q - q_0)\right).$$

These states are all unit normalized, $\|\psi_{\hbar}(q_0, p_0)\| = 1$. By formula (7) corresponding normalized Wigner function has the form

$$W_{\hbar}(x; q_0, p_0) = \frac{1}{(\pi\hbar)^n} \exp\left(-\frac{(q - q_0)^2 + (p - p_0)^2}{\hbar}\right).$$

Two important remarks should be made about this function.

Remark 1. Function $W_{\hbar}(x; x_0)$ is positive and thus can be interpreted as the classical statistical density.

Remark 2. In view of the following formula

$$\lim_{\hbar \rightarrow 0} W_{\hbar}(x; x_0) = \delta(x - x_0) \quad (17)$$

it is evident that the symbol of the quantizer $\Delta(x)$ is proportional to the limit of the sequence of Wigner functions $W_{\hbar}(x; x_0)$ of the localized Gaussian states as their width $\sqrt{\hbar}$ goes to 0.

Thus the \hbar -independent symbol $A(x_0)$ of an operator \hat{A} evaluated at point x_0 of the phase space appears as the mean value calculated with respect to the localized Gaussian state with parameters $x_0 = (q_0, p_0)$ in the limit when the width of the state goes to zero

$$\lim_{\hbar \rightarrow 0} \langle \psi_{\hbar}(q; x_0) | \hat{A} | \psi_{\hbar}(q; x_0) \rangle = \lim_{\hbar \rightarrow 0} \int A(x) W_{\hbar}(x; x_0) dx = A(x_0).$$

Note that this limiting process takes one outside the framework of quantum expectation values. The norm $\|\Delta(x)\| = 1$ implies that for any pure state $\hat{\rho} = |\psi\rangle\langle\psi|$

$$|\rho(x)| \leq 2^n \quad \text{and} \quad |W(x)| \leq \left(\frac{2}{\hbar}\right)^n. \quad (18)$$

This means that the quantizer or any singular symbol such as $\delta(x - x_0)$ does not correspond to a pure state. The global bound (18) forces $\rho(x)$ to be distributed in phase space without large peaks and is an evident consequence of the uncertainty principle.

Let quantum operator \hat{A} have Weyl symbol $A(x)$, and time dependent operator $\hat{A}(t) = U^+(t)\hat{A}U(t) = A(\hat{X}(t))$ has Weyl symbol $A(x, t; \hbar)$ such that $A(x, 0; 0) = A(x)$. Consider now the following expression

$$\langle A \rangle(t, x_0; \hbar, \varepsilon) = \int W_{\varepsilon}(x; x_0) A(x, t; \hbar) dx$$

as a function of two small parameters \hbar and ε . The following table shows meaning of the expression if one or both of the parameters are 0.

$\langle A \rangle(t, x_0; \hbar, \varepsilon)$	$\hbar \rightarrow 0$	$\hbar \neq 0$
$\varepsilon \rightarrow 0$	classical observable $A(x(t, x_0))$	symbol $A(x_0, t; \hbar)$ of quantum observable $\hat{A}(t)$
$\varepsilon \neq 0$	classical statistical mean $\int dy W_\varepsilon(y; x_0) A(x(t, y))$	quantum mechanical mean value

Note that function W_ε for $\varepsilon \neq \hbar$ does not correspond to a pure state $\psi(q)$, but rather is a density matrix.

4. Classical and quantum Lyapunov exponents.

From the table we see that the symbol $A(x_0, t; \hbar)$ is in fact quantum analog of the classical value $A(x(t, x_0))$. This is due to Egorov Theorem which states

$$\lim_{\hbar \rightarrow 0} A(x, t; \hbar) = A(x(t, x_0)), \quad (19)$$

where $x(t, x_0)$ is classical trajectory.

Thus the quantum analog of $(v \cdot \nabla_{x_0}) A(x(t, x_0))$ will be $(v \cdot \nabla_{x_0}) A(x_0, t; \hbar)$.

From the 1st formula of (10) one has

$$A(x_0, t; \hbar) = 2^n \int \langle q' | \Delta(x_0) | q'' \rangle \langle q'' | \hat{A}(t) | q' \rangle dq'' dq'.$$

Here we see that whole information about the point x_0 of phase space is contained in the quantizer kernel $\langle q' | \Delta(x_0) | q'' \rangle$. Thus the derivative $(v \cdot \nabla_{x_0})$ will only effect this part of the formula

$$(v \cdot \nabla_{x_0}) A(x_0, t; \hbar) = 2^n \int [(v \cdot \nabla_{x_0}) \langle q' | \Delta(x_0) | q'' \rangle] \langle q'' | \hat{A}(t) | q' \rangle dq'' dq'.$$

From (13) we obtain

$$2^n (v \cdot \nabla_{x_0}) \langle q' | \Delta(x_0) | q'' \rangle = \langle q' | \hat{\rho}_0^v | q'' \rangle,$$

where $\langle q' | \hat{\rho}_0^v | q'' \rangle$ is given by (6). So far we have

$$(v \cdot \nabla_{x_0}) A(x_0, t; \hbar) = \int \langle q' | \hat{\rho}_0^v | q'' \rangle \langle q'' | \hat{A}(t) | q' \rangle dq'' dq' = \langle \hat{A}(t) \rangle_{\rho_0^v} \quad (20)$$

Now, let $A(x)$ be a vector function. Introduce

$$\Lambda_v^A(x_0; \hbar) = \lim_{t \rightarrow \infty} \frac{1}{t} \ln ||(v \cdot \nabla_{x_0}) A(x_0, t; \hbar)||. \quad (21)$$

Using (20) we can also write

$$\Lambda_v^A(x_0; \hbar) = \lim_{t \rightarrow \infty} \frac{1}{t} \ln ||\langle \hat{A}(t) \rangle_{\rho_0^v}||. \quad (22)$$

Taking limit $\hbar \rightarrow 0$ in (21) we get

$$\Lambda_v^A(x_0; 0) = \lim_{t \rightarrow \infty} \frac{1}{t} \ln ||(v \cdot \nabla_{x_0}) A(x(t, x_0))||. \quad (23)$$

This formula is well defined for a wide class of vector functions $A(x)$. To get the classical Lyapunov exponent one must make however the special choice $A(x) = x$. Then formula (23) becomes exactly (1).

In the quantum case symbol $A(x) = x$ defines operator \hat{x} which makes it possible to talk about the *quantum trajectory* [3] defined as the symbol of $\hat{X}(t) = U^+(t)\hat{x}U(t)$

$$X(x_0, t; \hbar) = \lim_{\varepsilon \rightarrow 0} \text{Tr} \hat{X}(t) \hat{\rho}_\varepsilon = \lim_{\varepsilon \rightarrow 0} \int X(x, t; \hbar) W_\varepsilon(x; x_0) dx.$$

Then formula (22) gives us definition of the quantum Lyapunov exponent, which coincides with (5), (6).

In view of (19) $\lim_{\hbar \rightarrow 0} X(x_0, t; \hbar) = x(t, x_0)$, and the notion of quantum trajectory and (21), (22) allows also to write (5) in a form similar to (1)

$$\Lambda_v = \Lambda_v^X(x_0; \hbar) = \lim_{t \rightarrow \infty} \frac{1}{t} \ln \{(v \cdot \nabla_{x_0}) X(x_0, t; \hbar)\}. \quad (24)$$

5. Radon transform and tomographic procedure.

Let us make a few comments on the approach undertaken in [2]. To simplify exposition of some formulas and their geometrical meaning we assume in this section that $n = 1$, i.e $q \in \mathbb{R}^1$, $x \in \mathbb{R}^2$.

Although the integral of the Wigner function for the density matrix $|\psi\rangle\langle\psi|$ is always 1, typically there are regions in phase space where $W(x)$ is negative. This behavior results from the spectral expansion of the quantizer. Property 1 shows that the spectrum of $\Delta(x)$ is ± 1 for all x . In detail

$$\Delta(x) = P_+(x) - P_-(x), \quad I = P_+(x) + P_-(x) \quad (25)$$

where $P_\pm(x)$ are the spectral projectors for the eigenvalues ± 1 . If $x = 0$, then $\Delta(0)$ is parity operator on \mathcal{H} and $P_\pm(0)$ are the corresponding even and odd projectors. When $x \neq 0$ then $P_\pm(x)$ are the Heisenberg translates

of these operators, namely $T(x/2)^+ P_{\pm}(0)T(x/2)$. Applying (25) to $W(x)$ gives the Royer expansion

$$W(x) = \frac{2}{h} [||P_+(x)\psi||^2 - ||P_-(x)\psi||^2] .$$

So whenever $||P_+(x)\psi|| < ||P_-(x)\psi||$ then $W(x)$ is negative. This makes it impossible to interpret it as a classical statistical density.

Nevertheless the two physically important *projections* of the $W(x)$, namely

$$\int W(q, p) dp = |\psi(q)|^2 , \quad \int W(q, p) dq = |\tilde{\psi}(p)|^2$$

are positive and form corresponding marginal distributions. Here $\tilde{\psi}(p) = h^{-n/2} \int \psi(q) e^{-ipq/\hbar} dq$ is the wave function in the momentum representation.

One may consider a family of *projections* with respect to all directions, in the phase space, not only the two given above. In this way we obtain Radon transform of $W(x)$

$$RW(Q, \xi, \eta) = \int W(q, p) \delta(Q - q\xi - p\eta) dq dp .$$

Here $Q - q\xi - p\eta = 0$ is an equation of line in the phase space. Rewriting the above formula as

$$\begin{aligned} RW(Q, \xi, \eta) &= \frac{1}{2\pi} \int W(q, p) e^{-ik(Q - q\xi - p\eta)} dk dq dp \\ &= \frac{1}{2\pi} \int dk e^{-ikQ} \int dq dp W(q, p) e^{i(kq\xi + kp\eta)} \end{aligned}$$

one can see two remarkable things. First, the RHS can be viewed as a inverse Fourier of a characteristic function $\int W(q, p) \exp\{i(kq\xi + kp\eta)\} dq dp$ and thus is non-negative and represents a marginal distribution. Second, Radon transform is a composition of 2D-Fourier transform and 1D-inverse Fourier transform, thus it is invertible. The inverse Radon transform can be written as

$$W(q, p) = \int dQ d\xi d\eta RW(Q, \xi, \eta) e^{i(Q - q\xi - p\eta)} .$$

This means that knowing *projections* in all directions one can reconstruct $W(x)$ from them by the inverse Radon transform. This property is widely used in computer tomography.

Due to invertibility of Radon transform the tomographic representation is equivalent to Weyl symbols representation. In particular the formula for the quantum mean takes form (4)

$$\langle \hat{A} \rangle_\rho = \int dx A(x)W(x) = \int dQ d\xi d\eta \tilde{A}(\xi, \eta) RW(Q, \xi, \eta) e^{iQ},$$

where $\tilde{A}(\xi, \eta)$ is inverse Fourier of $A(q, p)$, and $RW(Q, \xi, \eta)$ is the tomographic distribution corresponding to $W(x)$.

Any of these representations finally lead to the same formula for the quantum Lyapunov exponent.

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